

The LLNL Simulation Environment

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ICCD Development Environment
Group
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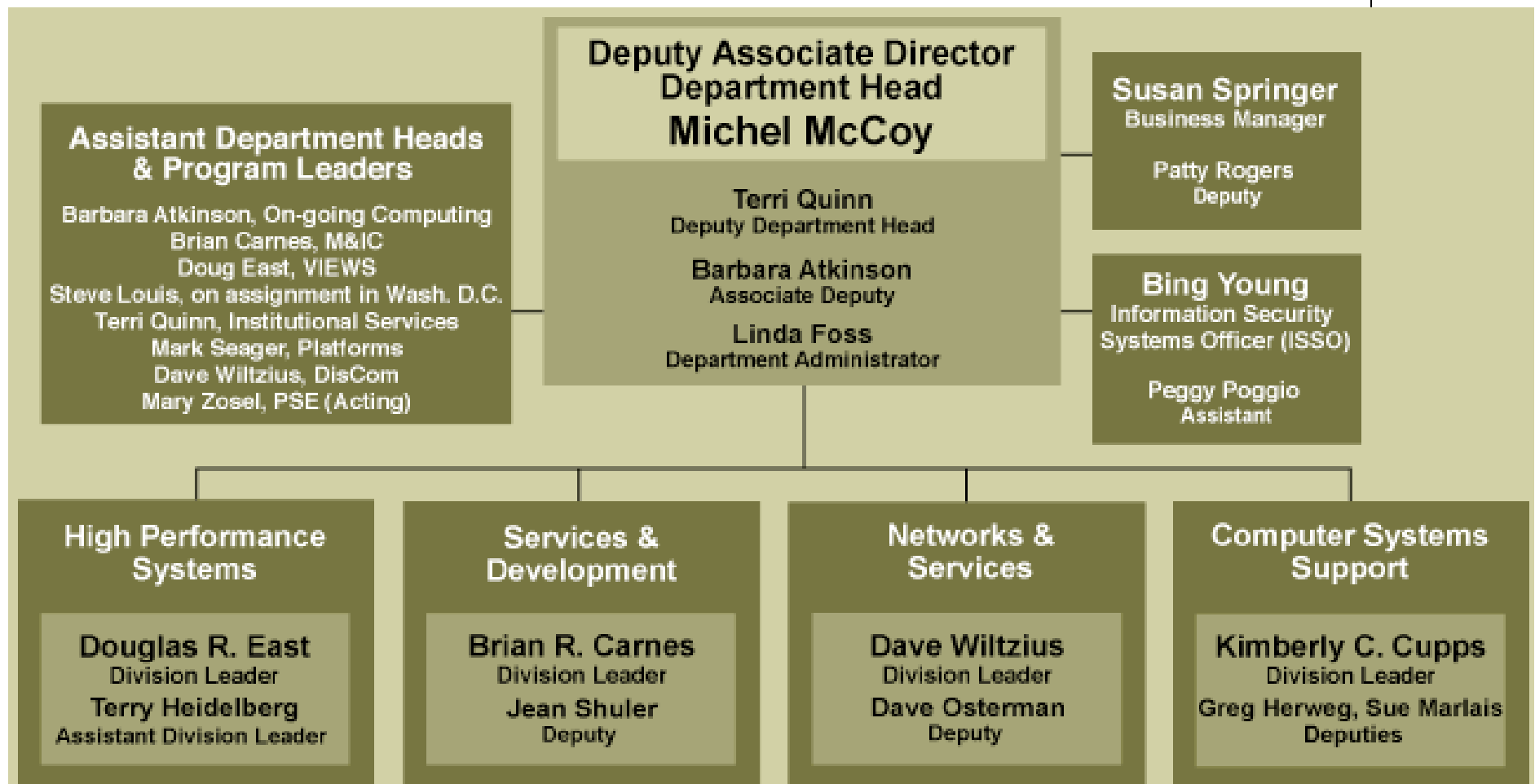


Overview

- The LLNL code development environment for the BlueGene/L simulator
 - General Livermore Computing (LC) user support structure
 - LC compute resources for running the BlueGene/L simulator
 - BGL simulator status at LLNL
 - Compute environment issues- compilers, libraries, debugging
 - Available support for BlueGene/L simulator and apps development
 - Access and availability for alliance partners and LLNL teams



ICCD Organizational Structure



Services and Development Division provides the user support infrastructure



Division Leader
Brian R. Carnes

Jean Shuler
Deputy Division Leader

Computation Training Center

Sue Wiebe
Manager
Diane Couch
Training Center Coordinator

Customer Services Group
Jean Shuler
Group Leader

Account Management
Team Lead: Chris Garcia

4-Help Desk
Team Lead: Sue Wolfe

HPC Hotline
Team Lead: Babara Herron

Blank, Ben
Brewer, Sandra
Carnes, Jeanette
Castle, Rene
D'Hooge, Michelle
Dannenberg, David
Delpha, Teresa
Hadjimarkos, Stella
Hargreaves, Charlie
Harlan, Louise
Hill, Bruce
Hindmarsh, Alan
Huerta, Rena
Molyneaux, Brian
Nemanic, Michael
Reed, Aileen
Revelli, JoAnne
Russell, Angeline
Walraven, Jason

Special Projects
Web Design and Support
Documentation
Training
Jean Shuler, Group Leader
Barney, Blaise
Gebur, Elizabeth
Girill, Terry
Jenness, Jeanette
Wong, Lori

Development Environment
Scott Futral
Group Leader

Ahn, Dong
Chambreau, Christopher
Chan, Bor
Engle, John
Gyllenhaal, John
Hedges, Richard
Jones, Terry
Loewe, William
Morrone, Christopher
Mclarty, Tyce
Shereda, Charles
Stanberry, Linda
Warren, Karen
Wolfe, Matt

**Integrated Computational
Resource Management**
Greg P. Tomaschke
Group Leader

Eckert, Philip
Harding, Charles
Hommes, Gregg
Jette, Morris
Lipari, Don
Pezzone, Amy
Wood, Robert
Yoo, Byung Suk (Andy)

**Information Management
and Graphics**
Rebecca Springmeyer
Group Leader

Ahern, Sean
Arrighi, Bill
Blair, Mark
Bremer, David
Cook, Richard
Cronshagen, Eugene
Foote, Betsy
Frank, Randy
Gaunt, Ross
Jones, Holger
Krauss, Liam
Long, Jeffery
Miller, Scott
Newton, Ramon
O'Neill, Neil
Prevost, Shelly
Rowe, Jeffery
Smith, Neale
Spencer, Paul

Customer Services and Support Group is the first contact point for users

lc-hotline@llnl.gov 925-422-4532



- Hotline Call Centers
- Information dissemination
- Education and training
- Problem reporting, tracking, and resolution
- Customer outreach
- 24x7 customer support

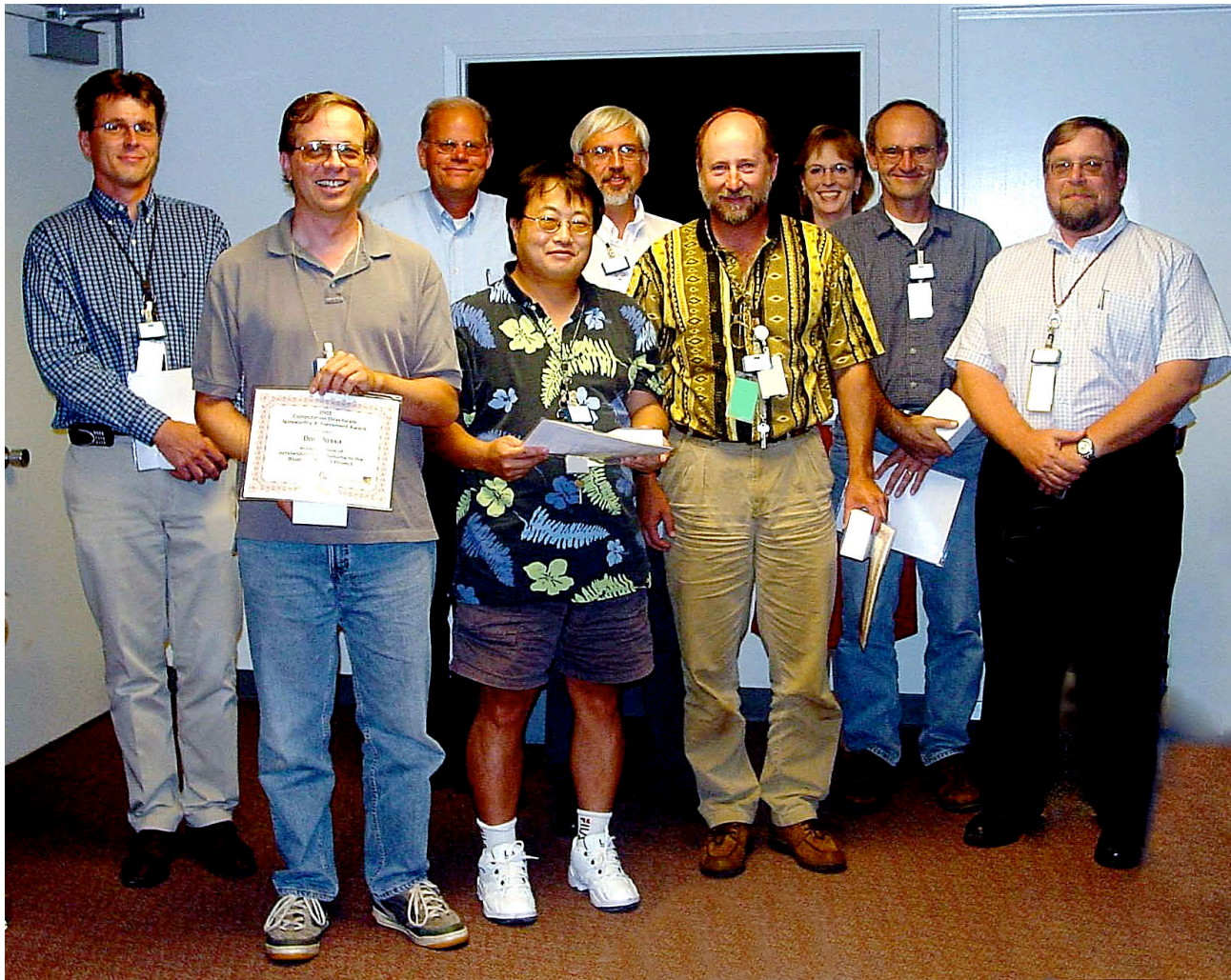


CSSG staff members at work in LC's Hotline

CSSG leverages the expertise of other ICCD groups to enhance the breadth of customer support

**Operations ♦ Development Environment ♦ Information Management and Graphics
High Performance Computing ♦ Distributed Computing ♦ Storage ♦ CASC ♦ Network**

BGL and BGLsim expertise at LLNL currently resides in CAR/CASC. ICCD support will leverage this resource.



Pictured are selected members of the LLNL Computation-Directorate BlueGene/L team (left to right):

Francois Gygi, Don Dossa, Mark Seager, Andy Yoo, Kim Yates, Bruce Curtis, Dona Crawford, Tim Pierce, Lynn Kissel

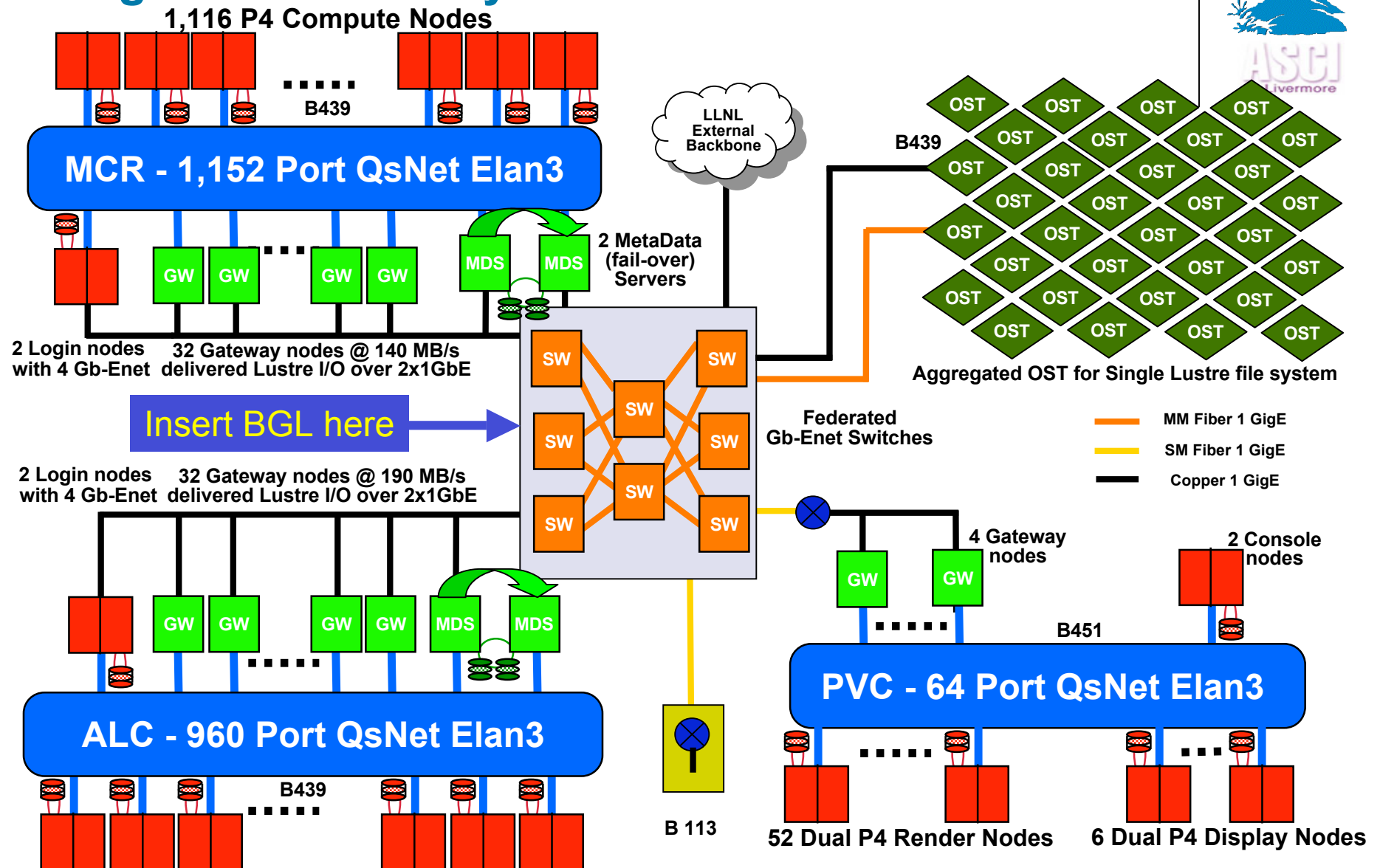
Not pictured:

Bronis de Supinski, Jeff Vetter, Bor Chan, Scott Banachowski

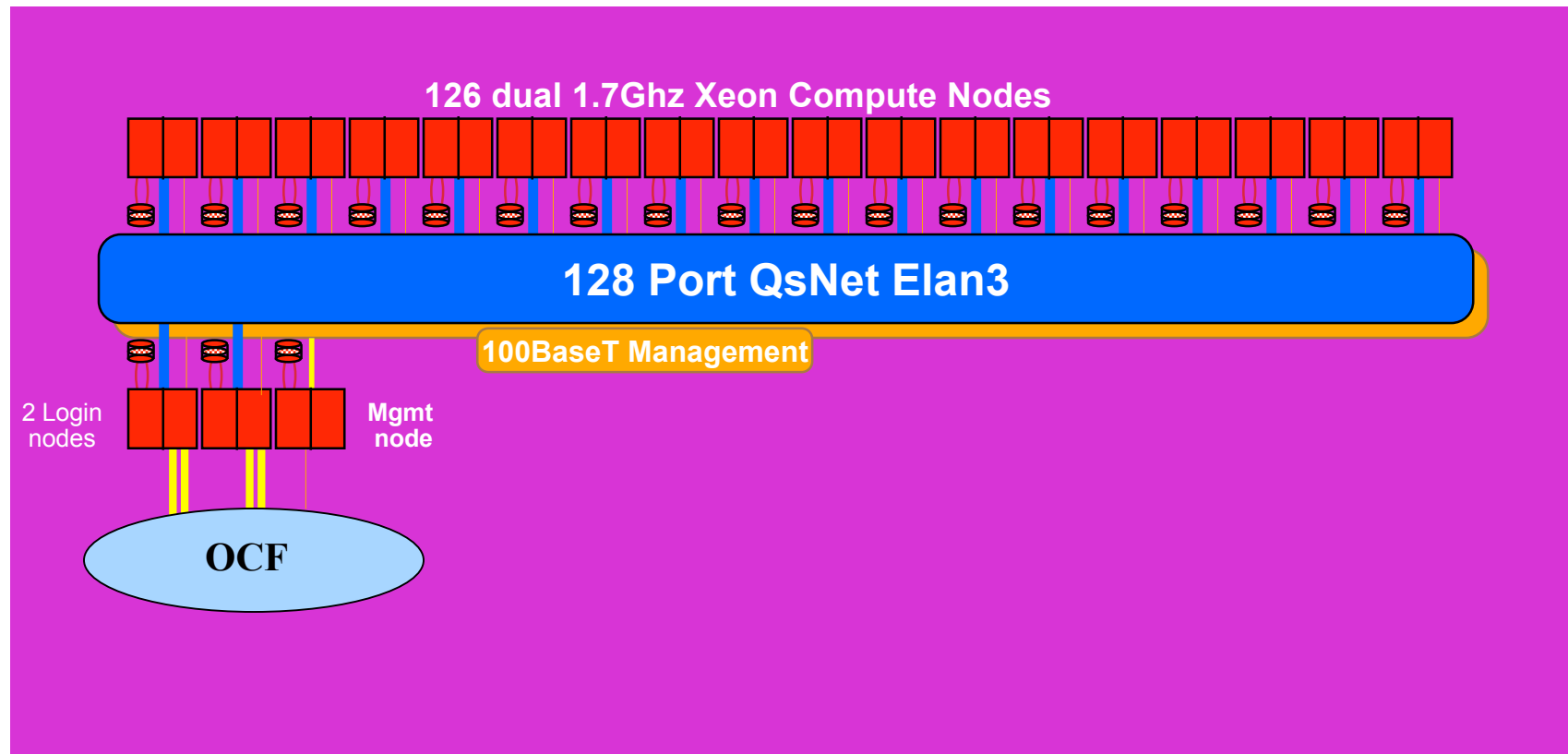
First-wave applications:

Andy Cook, Bill Cabot, Francois Gygi, Jack Reaugh, Jeff Greenough, Rob Neely, Wei Cai

Multi-cluster Simulation Environment based on a single Lustre File System at LLNL



BGLdev (or bigdev) is intended for BlueGene/L applications development. Expected availability in mid-November.





The BlueGene/L simulator is installed and functional on ALC

- BG/L Sim has been ported to the LLNL IA32/Quadrics systems, and is installed on ALC
- Modifications were made to enable over MPICH, some legacies apparent such as SIMBOOT_MACHINES
- /BlueLight/floor directory contains cross compilers
- /BlueLight/lnl_2003-09-23 has the BG/L runtime and examples
- The simulator mounts /bgl file system
- Notes and examples of usage will be posted to the BG/L web site- <www.llnl.gov/asci/platforms/bluegenel>



BG/L sim code development environment

- Currently, only Gnu compilers are available on ALC.
- No support for double hummer in the Gnu compiler.
- Gnu Fortran is generally recognized as inadequate.
- IBM XL compilers are expected to be made available on site- can be accessed at IBM ihost site.
- Debugging? See Totalview talk at 2:30. Printf is the current status.
- Common apps libraries need to be identified and made available: Silo, LEOS, Hypre, ESSL,...

First-wave applications identified- ~.5 FTE support allocated per team for BG/L dev



- GP, first-principles molecular dynamics, Francois Gygi
- DD3d, dislocation dynamics, Wai Cai, Tim Pierce
- ALE3D, high-explosives modeling, Jack Reaugh, Rob Neely
- Miranda, turbulence, Andy Cook, Bill Cabot
- Raptor, computational fluid dynamics, Jeff Greenough
- Additional personnel have been identified for BG/L support.



ALC access is highly contentious with competing demands for resources

- Lustre file system testing for multinodes
- Lustre IGS file system testing
- New Lustre version release testing
- CFS additional Lustre work requires FN access, creating issues for export controlled codes.
- ASCI Alliances expect a significant time allocation
- LLNL ASCI users expect access
- BG/L file system scaling effort
- BG/L simulation effort



Brian Carnes' proposal for ALC allocation

- Split the machine in two most of the time, with dedicated full machine runs (DAT) available by request
- Lustre related efforts would have 480 nodes and 52 TB /p/ga2 file system
- BGL Simulation and ASCI Apps efforts will share 480 nodes and 21 TB /p/ga1 file system
- DAT requests handled in Thursday meeting for 4pm Friday to 8am Monday session.
- Extended week-long DAT available when warranted.
- ALC accounts to be requested through normal LC-support forms, and approved by Carnes or other LC management.
- Will be available after file system reconfiguration, ~ 2 weeks.



BGLdev will be needed too!

- BGLdev will be configured so as to permit access for sensitive codes.
- No root access for foreign nationals.
- BGLdev will help with simulator access during DAT or peak demand times.
- BGLdev accounts will be requested through LC-support, with approval by appropriate LC/Comp management.



Summary

- BlueGene/L Simulator is available at LLNL
 - Currently installed on ALC
 - A dedicated 'BGLdev' cluster is in the works
- ICCD/Livermore Computing and CAR/CASC will support the applications development teams
 - 2 FTE's are allocated for helping apps teams
 - LC support infrastructure in place for ALC and BGLdev